Design of a Microfluidic System in a PEMFC Cell

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ABSTRACT

In this paper, it is presented the design and simulation of a prototype proton exchange fuel cell (PEMFC) micro scale with the ultimate goal of providing electricity in mobile applications which are almost indispensable in our daily use development. A numerical analysis was done by simulating computational fluid dynamics flow field using the COMSOL Multiphysics software, taking into consideration that our fluid flow with a physical model of creeping flow (Re <400), with which reached analysis to find the pressure distribution and flow rate within two proposals flow plate coil geometric arrangement, concluding that would be used for further study of the proposals, the cell that is located a discarded pressure drop due to the arrangement of the flow plate, thereby achieving optimal distribution of the reagents on the active surface of the fuel cell to the proposed scale.

Taking the final proposal plate electrochemical flow analysis was performed, making the assembly of the physical model using physical Secondary Current Distribution (SIEC) to assess the conservation of electric charge inside the cell and to evaluate conservation physical model species Reactive Flow in Porous Media (RFCs) for anode and cathode. To evaluate the electrical performance of the polarization curves given fuel cell were obtained, i.e. the graph cathode electric potential depending on the electric current density and the graph of the electrical power density based on the density electric current, with which the result and efficiency compared with the theoretical curve of a PEMFC cell polarization observed that achieved by the simulation results shown are acceptable.

Keywords—Proton exchange fuel cell (PEMFC), creeping flow, Secondary Current Distribution (SIEC), Reactive Flow in Porous Media (RFCs)

I. INTRODUCTION

The search for new sources of clean energy and replace fossil sources use has been extensively studied in recent decades (1). Considering fuel cells as a source of clean energy generation, we have many choices within the same frame: (alkali fuel cell, AFC, phosphoric acid, PAF, molten carbonate, MCFC, solid oxide SOFC) (2), in this paper proton exchange membrane is considered, PEMFC. PEMFC is considered one of the cells with greater efficiency for mobile devices, as it works at low temperatures (40-80 °C), can use oxygen as fuel and high current density (1) compared to electrochemical cells business.

With the aim of mobile applications in the past decade there have been efforts for technological research to release a miniaturization and thereby improve the electrochemical performance (3). For PEMFC mobile application as already mentioned, it is important to generate high current densities which can achieve adequate hydration of the membrane, the distribution of reagents and materials that make the (4; 5; 6; 7; 8), among other conditions.

Computational fluid dynamics (CFD) has become a powerful tool for the simulation and optimization of fuel cells, allowing us a good fit between the physical operation involving, as is the distribution of anode current and cathode transport of species between porous media (5) and thereby achieve an improvement in future models.

The research focuses on the design of a microfluidic system in a PEMF cell, for which is considered important for the performance of it by changing the geometry several studies have been conducted on this topic: parallel and interdigitated flow arrangements, serpentine shape (9; 10; 11; 12; 13; 14), more complex designs such as the Sierpinski (circular shape) (15) and the Hilbert fractal shape (16). The geometric arrangement showing better performance is the serpentine in which we are working with, as it has a better distribution of reactive and therefore its consumption also in water management is improved with this arrangement (17).

Taking into account the literature on the geometrical arrangement of flow plates will start with two settlement proposals serpentine, with the difference between each start for the distribution of reagents within them, using elbow 90 in one and the other radial side, showing by this
falling pressure and thereby determine pressure drops within them, having chosen a final proposal is reached the electrochemical analysis and obtain the polarization curves of the cell.

The structure of the article is as follows: in the second section will be given a description and modeling of PEMFC, in the third section the model results and conclusions are presented.

II. METHODOLOGY

In Fig. 1, the composition of the two proposals micro PEMFC, which consist of 6 layers each shown. Prototypes are drawn using SolidWorks® as shown listed: 1 and 6, flow plate engraved in a polymer " Polymethyl methacrylate " with a depth of 300μm and 300μm width; 2 anode gas diffusion layer of carbon paper hydrophobic with no less than 200μm thick; 3 catalyst plate formed by a plate load of 0.5 mg/cm²; 4 perfluorosulfonada Nafion® 117 membrane with a thickness of 180μm; 5, cathode gas diffusion layer of hydrophobic carbon paper weighing less than 200μm thick.

Fig. 1 Isometric view of a cell PEM a) 90° elbow serpentine shape, b) radial elbow serpentine shape.

The flow plate has 17 channels, the channel to rib ratio CR = 1, i.e. the channel and the width of post is 300μm, aspect ratio AR = 1, the active area of the plate flow A = 1cm², electronic conduction area is 0.5 cm², the total length of the channels is L=162mm, for the hydraulic connection commercial stainless steel needle of 0.8 mm diameter are used.

Influencing phenomena involved in the operation of the PEMFC are mass transport of different species (H₂, O₂, H₂O, N₂), fluid flow, the electrochemical reaction and heat transfer.

To make the mathematical model are partial differential equations that describe the phenomena described above, for which the following assumptions are made:

- isometric materials,
- isothermal behavior,
- laminar flow (Re<400),
- incompressible flow.

2.1 Hydrodynamic Considerations

In the analysis and design of the plates the hydrodynamic analysis was performed, considering that the size of the channels is comparable with, λ, mean free path of the gas molecules with the Knudsen number, Kn, determine the degree of thinning of gas, and the characteristic length, L, which is equal to the hydraulic diameter, D_h, (18) the above terms can relate to the Eq. 1 (19):

\[ Kn = \frac{\lambda}{L} \]  

(1)

To calculate the number of Knudsen you can get from the logarithmic plot of the Knudsen number based on the hydraulic diameter of microchannels different shown in Fig. 2 (20):

![Fig 2 Log plot Knudsen number based on the hydraulic diameter of microchannels different.](image)

In conventional thermodynamic systems in which gas at standard conditions of temperature and pressure are used, the characteristic length is much greater average free path of the gas, and the Knudsen number is essentially zero. For such systems, the physical domain is large compared with the mean free path of the fluid, L >> λ, for which can be seen as an ongoing matter where their local properties can be determined from the averaged value of the molecular properties such as mass, velocity and energy.

2.2 Governing differential equations

To start with the equations governing the model of micro-PEMFC, we have the following conservation equations: Eq. 2 of conservation of mass and Eq. 3 Momentum conservation.
\[ \nabla \cdot \mathbf{u} = \frac{Q}{\rho} \]  (2)

\[ \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \left( -pI + \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] \right) \]  (3)

Where \( \mathbf{u} \) is the velocity of the gas mixture (m/s), \( \rho \) is the mixture density (kg/m\(^3\)), \( Q \) is the source term (kg/m\(^3\)s), \( p \) is the pressure (N/m\(^2\)), and \( \mu \) is the dynamic viscosity of the mixture (kg/m s) which is calculated using Eq. 4 (21):

\[ \mu = \sum_{i} x_i \mu_i \]  (4)

In the gas diffusion layer (GDL), the pressure drop is proportional to the gas velocity if the flow is laminar, and is modeled as Eq. 5 (21):

\[ \left( \mu / \kappa \right) \mathbf{u} = \nabla \left( -pI + \left( 1 / \varepsilon \right) \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] \right) \]  (51)

Where \( \kappa \) is the permeability of the GDL (m\(^2\)) and \( \varepsilon \), is the porosity of the GDL.

Multispecies mass transport is in whole computational domain, including flow channels and gas diffusion layer which are described by the Stefan-Maxwell equation. Which resolves flows in terms of mass fraction. The general form of the Stefan-Maxwell equation shown in Eq. 6 (21).

\[ \nabla \left\{ -\rho w_i \sum_{j=1}^{N} D_{ij} \left[ \frac{M_j}{M} \left( \nabla w_j + w_j \frac{\nabla M}{M} \right) + \left( x_j + w_j \right) \nabla P \right] + w_i \rho \tilde{u} \right\} = R_i \]  (6)

Where \( D_{ij} \) is the binary diffusion coefficient, \( x \), is the mole fraction, \( w \), is the mass fraction, \( M \), is the molar mass, \( R \), is the universal gas constant (8.314 J/mol K), \( T \), is the operating temperature of the cell (K), \( \rho \), it is the density of the gas mixture, which is described by Eq. 7 (21).

\[ \rho = \left( \sum_{i} x_i \mu_i \right) P / (R \cdot T) \]  (7)

Subscripts \( i \) and \( j \) represent different species, \( R_i \) is the reaction rate, which explains reagent consumption and product production during the electrochemical reactions in the catalyst layer, for calculating the \( R_i \) is used Eq. 8 (21).

\[ R_{H_2} = -\frac{j_a}{2F} M_{H_2} \]
\[ R_{O_2} = -\frac{|j_e|}{4F} M_{O_2} \]
\[ R_{H_2O} = -\frac{|j_e|}{2F} M_{H_2O} \]  (8)

On the cathode side, only the oxygen and water mass fraction is replaced, since the third species can always be obtained from mass balance Eq. 9 (21).

\[ w_{N_2} = 1 - w_{O_2} - w_{H_2O} \]  (9)

On the anode side, the mass fraction of hydrogen thereby obtain the mass fraction of water as is used Eq. 10 (21).

\[ w_{H_2O} = 1 - w_{H_2} \]  (10)

The \( D_{ij} \) binary diffusion coefficient used in the Stefan-Maxwell equation is calculated from an empirical correlation with Eq. 11 (22).

\[ D_{ij} = D_{ij,0} \left( \frac{T}{T_0} \right)^{1.5} \]  (11)

Where \( T_0 \) is the reference temperature and \( D_{ij,0} \) is the binary diffusion coefficient reference. In porous media binary effective diffusion coefficient amending Eq. 12 to take into account the effect of the porosity of the GDL, is calculated with Eq. 12 (23).

\[ D_{ij} = D_{ij,0} \varepsilon^{1.5} \]  (12)
In a PEMFC, the current can be divided into two parts: ion current and the electron current. When protons travel through the membrane to form an ion current, while the electrons are transferred only through the solid matrix of electrodes, which is an electronic current. The current continuity equations are obtained using Ohm's law, which is in Eq. 13 (21).

\[
\nabla \times (-\sigma_s \nabla \phi_s) = S_s \\
\nabla \times (-\sigma_m \nabla \phi_m) = S_m
\]

Where \( \phi_s \) is the potential phase, \( \sigma \) is the effective conductivity \( (S/m) \), \( S \) is the density of volumetric flow rate \( (A/m^3) \), the subscript \( s \) indicates the characteristic of the solid phase while \( m \), the membrane. The terms equations based on electron and proton transport are the result of the electrochemical reaction, which occurs only in the catalyst layers of both anode and cathode, and are obtained with Eq. 14 (21).

**Catalyst layer anode** \( S_m = j_a \)  
**Catalyst layer cathode** \( S_m = j_c \)

Where \( j_a \) and \( j_c \) are the current density transfer corresponding to the electrochemical reaction in the catalyst layers of the anode and cathode, respectively.

The source terms in both species and load equations are related to the current density transfer \( (j_a \) and \( j_c) \) and is calculated by Eq. 15 and Eq. 16, the Butler-Volmer equation (21).

\[

j_a = a_i^{ref} \left( \frac{C_{H_2}}{C_{H_2}^{ref}} \right)^{0.5} \left( \frac{\alpha_a + \alpha_c}{RT} \right) \frac{F\eta_a}{n_a}
\]

\[

j_c = a_i^{ref} \left( \frac{C_{O_2}}{C_{O_2}^{ref}} \right) \exp \left( -\frac{\alpha_c}{RT} \right) F\eta_c
\]

Where \( \eta \) represents the power differential between the solid matrix and the electrolyte and is defined by Eq. 17 (21).

\[

Anode: \eta_a = \phi_s - \phi_e \\
Cathode: \eta_c = \phi_s - \phi_e - U_{oc}
\]

## 2.3 Computational Method

To solve the above equations numerically, it was used COMSOL Multiphysics® software, which based its solution in finite element computer model discretizing the elementary volumes. The mesh of the computational model was performed using a structured mesh, using a free tetrahedral for the section of the channels, making a refined corners because elbows of geometry, to the remaining section a type of triangular mesh free was used because geometry has less complexity (see Fig. 3).

![Fig. 3 Isometric view of structured mesh, a) 114273 elements 90° elbow serpentine shape b) 466 061 elements radial elbow serpentine shape.](image)

## 2.4 Boundary conditions and initial

For operation of the cell, it has an inlet volumetric flow rate of \( 1.667{E^{-7}} \) m\(^3\)/s applied to \( H_2 \) and \( O_2 \). \( H_2 \) a mass fraction of 0.8 at the anode, to \( O_2 \) and \( H_2O \) respectively 0.2 and 0.1 in the cathode. A pressure of 1 atmosphere, at 27 \( ^\circ \)C it has which are operating conditions of the cell.

## V. CONCLUSION

Using the parameters and properties as mentioned above (geometry and materials), the pressure distribution analysis was performed on the section of the channels, using a volumetric flow \( Q = 10 \) ml/min, which is the influence of known form of settlement between the coil forms (elbow 90 degrees and radial elbow). These results are not considered electrochemical reactions.

In Fig. 4 the distribution of pressure (static) in the channels, in which one can observe the scale contours shown the static pressure gradient (a) was 2215-0 Pa and if (b) it was to 2186-0 Pa, applying greater pressure drop in (a) unlike (b) with which we can conclude that the pressure...
drop can provoke flooded channels, would affect FC performance.

In the analysis of the dynamic pressure, the pressure gradient (a) a zero pressure drop is observed at the corners of the model, furthermore a more stable pressure within the channel (b) behavior were reported (see Fig. 5).

With this study of pressure distribution within a single cell is conclusive determining geometry where the pressure drop is less, being part plate flows critical to the performance of the cell.

When choosing a suitable geometric arrangement we will ensure that the reagents within the cell ARE as long as possible within the same and that is made more effective chemical reactions.

Fig. 4 Contours of static pressure a) 90° elbow serpentine shape b) radial elbow serpentine shape.

Fig. 5 Contours of dynamic pressure a) 90° elbow serpentine shape b) radial elbow serpentine shape.

REFERENCES


